

LA-UR- 02-5071

Approved for public release;
distribution is unlimited.

C.1

Title: CartaBlanca-Rapid Prototyping Development Environment
for Non-Linear Systems on Unstructured Grids

Author(s): W. B. VanderHeyden, T-3, LANL
D. Livescu, T-3, LANL
N. T. Padial-Collins, T-3, LANL

Submitted to: ASCI Solvers Meeting, August 12-15, 2002, Monterey, CA



Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the University of California for the U.S. Department of Energy under contract W-7405-ENG-36. By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

Form 836 (8/00)

CartaBlanca- Rapid Prototyping Development Environment for Non-linear Systems on Unstructured Grids

Abstract

This talk describes a component-based nonlinear physical system simulation prototyping package written entirely in Java using object-oriented design. The package provides scientists and engineers a "developer-friendly" software environment for large-scale computational algorithm and physical model development. The software design centers on the Jacobian-Free Newton-Krylov solution method surrounding a finite-volume treatment of conservation equations. This enables a clean component-like implementation. We first provide motivation for the development of the software and then discuss software structure. Discussion includes a description of the use of Java's built-in thread facility that enables parallel, shared-memory computations on a wide variety of unstructured grids with triangular, quadrilateral, tetrahedral and hexahedral elements. We also discuss the use of Java's inheritance mechanism in the construction of a hierarchy of physics systems objects and linear and nonlinear solver objects that simplify development and foster software re-use. Following this, we show results from example calculations and then discuss plans including the extension of the software to distributed memory computer systems.

Objectives

- *Developer-friendly* rapid proto-typing tool.
- OO Java + Jacobian-Free Newton-Krylov + finite volume method
=> non-linear solver environment.
- Multiphase flow on unstructured grids for complex multi-material applications.
- Explore Java's thread facility and DSM's for parallel computations.

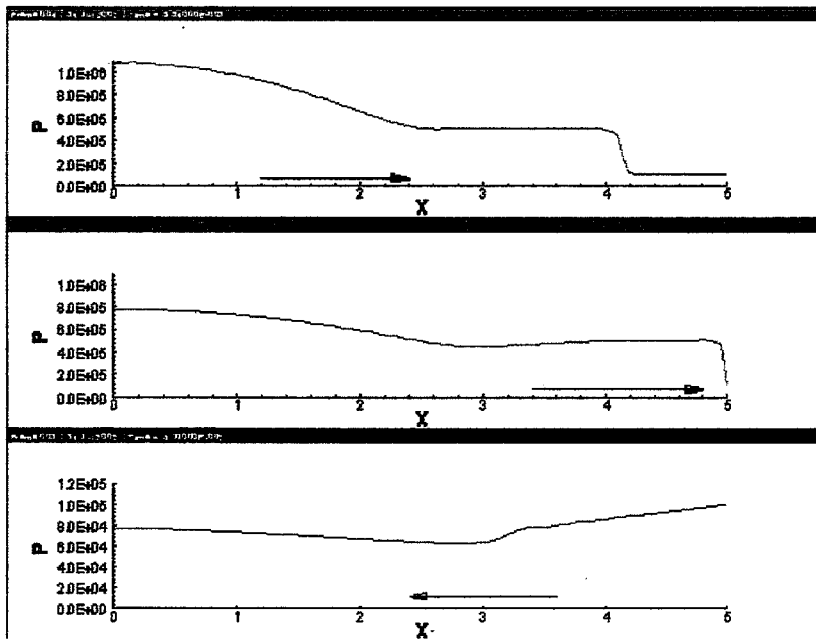
Why Java?

- Type-safe
- Safe memory model
- Object oriented programming
- Portable
- Large marketplace presence
- Many reusable components available
- Built-in threads for parallel, DSM's, ...

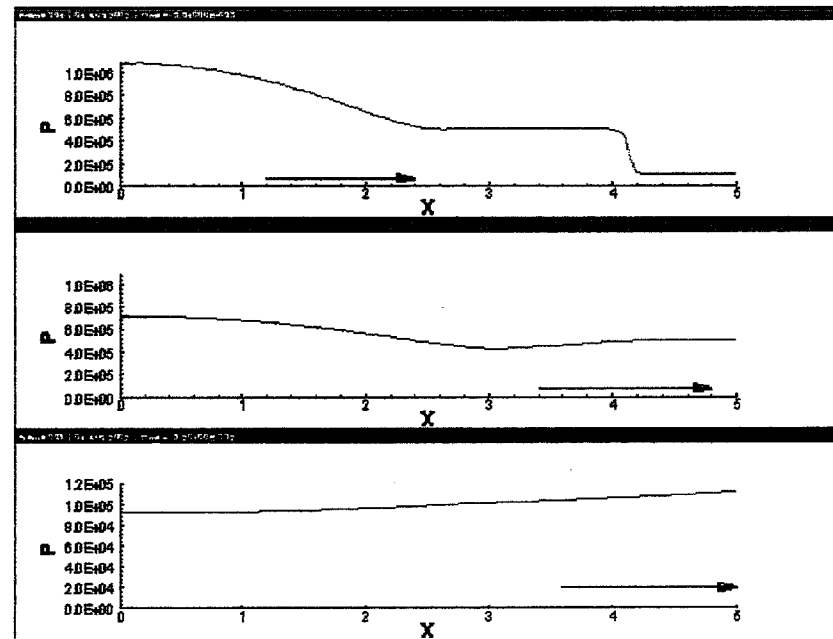
Compressible Flow

- Mach 3 Pressure wave.
- Effect of BC treatment.

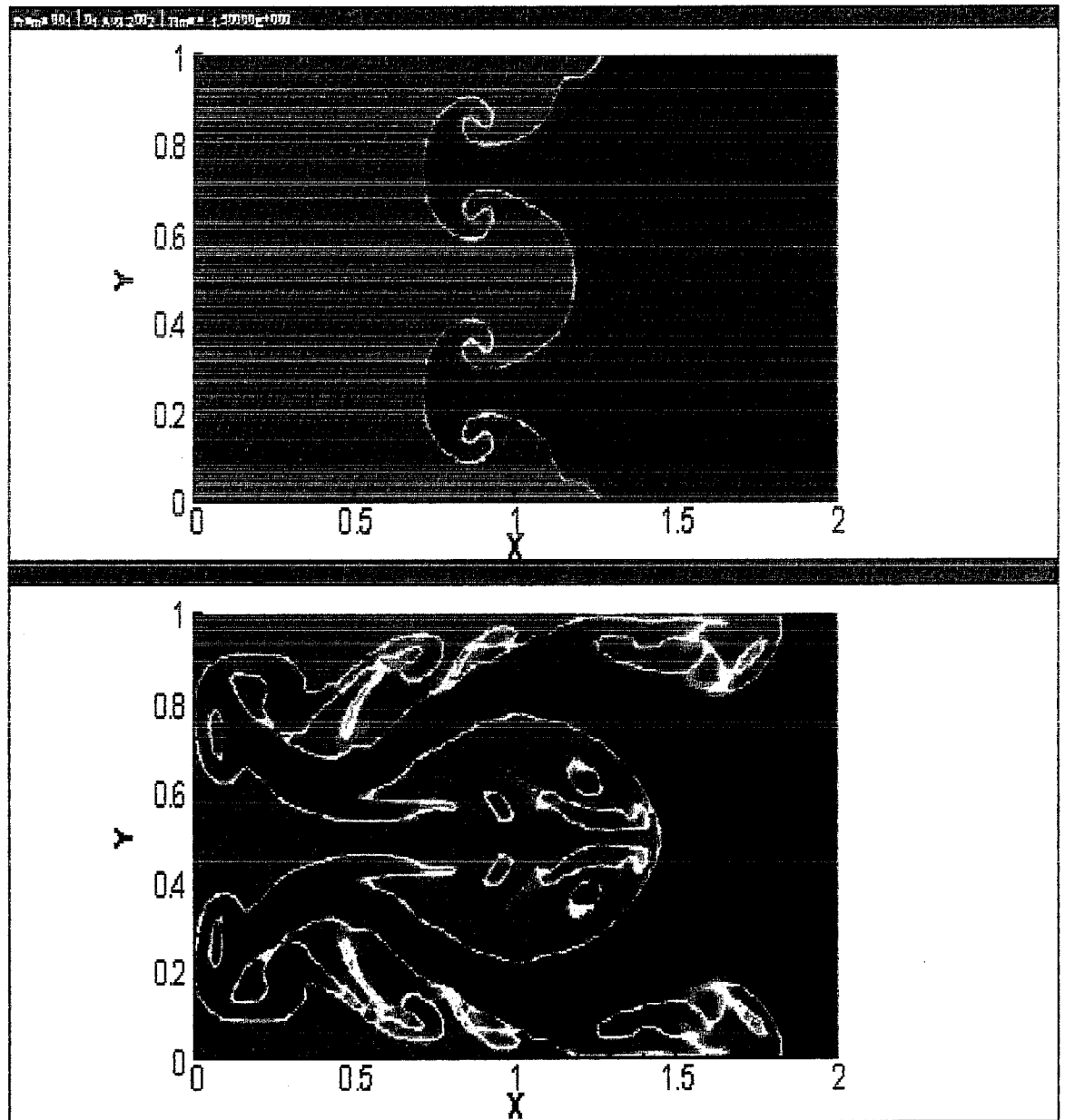
Constant pressure



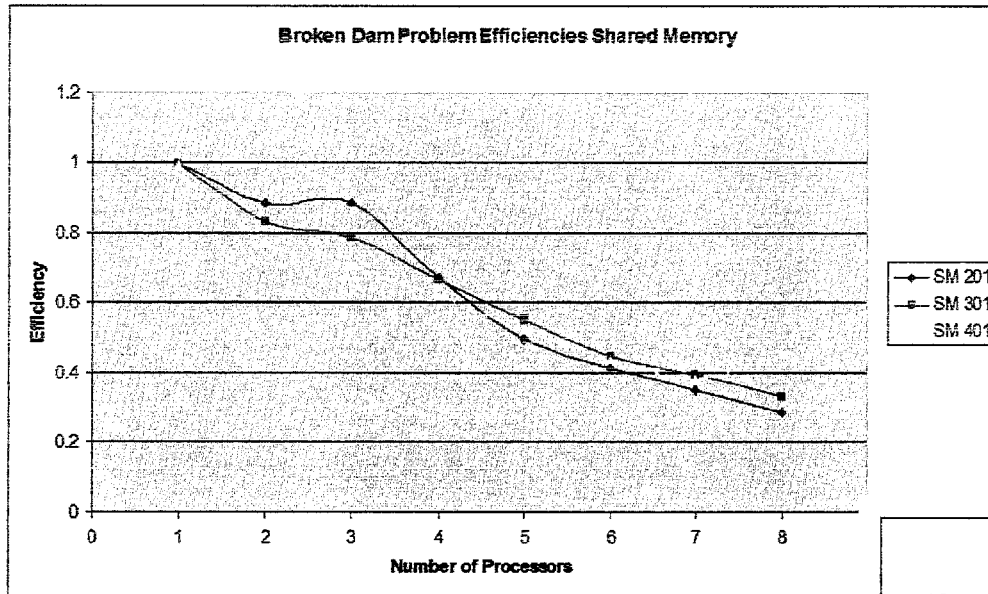
Non-reflecting



Compressible Rayleigh- Taylor Flow with Interface Tracking

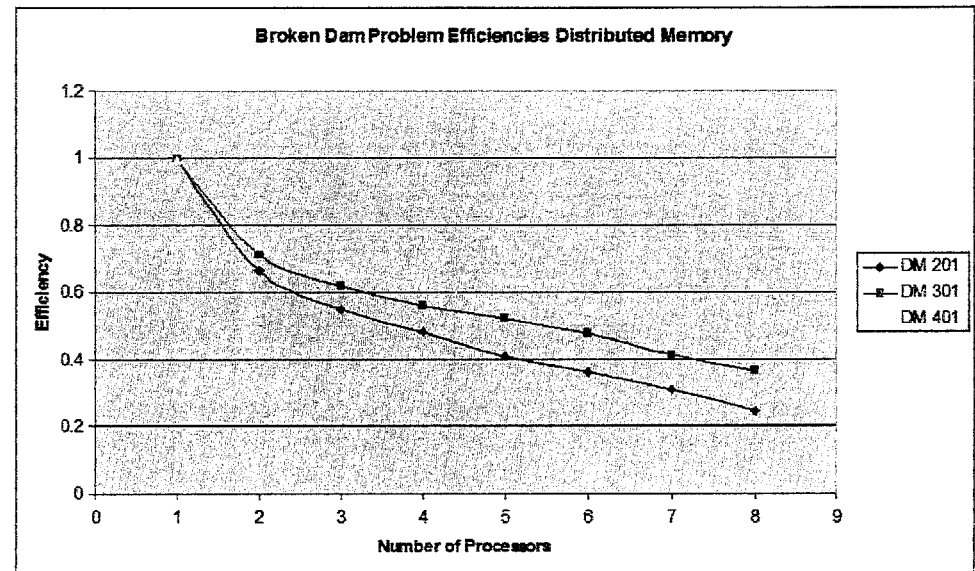


Scaling – Broken Dam Problem



Shared Memory

Distributed Memory
with JavaParty



Conclusions

- CB effectively combines NK and OO Java.
- In-function left preconditioning for inter-field preconditioning effective and convenient.
- Non-equilibrium phase changing multiphase flow demonstrated.